

65461

462

4 E 12

If more than one search is submitted, please prioritize searches in order of need.

72. Key: YC12 R₂ NT LAMINO BENZOIC ACID OR ALKOXY CARBONYL
Title of Invention: AMINO TETRAZOLYL PHENYL DERIVATIVES AS
IP ANTICANCERISTS
Inventors (please provide full names):

FRANCISCO JAVIER LOPEZ-TAPIA et al

Earliest Priority Filing Date: 3/2/2001

appropriate serial number.

(R)-or
Het-2

Aryl
or
Het-1

$\text{CH}_2\text{-O-CO-N} \begin{array}{c} \text{C}_6\text{H}_4 \\ \text{(R)} \end{array} \text{(CH}_2\text{)}_n\text{-X}$

X = -COOH
or

Het-1 \equiv

Het-2 = Pyridine / Pyrimidine / Thienyl / Pyrroline
or Pyrazine

R \equiv H / Alkyl / Halogen
or NO₂ / NH₂ / CN / Alkoxy
or Phenyl / -oPhenyl / Heterocycle

Need info from compounds / components / articles
Typical ANDIN IP into generic
Copy claim under

RECEIVED
MAR 26 1987

P=N
of CH₃

TITX
pyrrole
+ 624

Vendors and cost where applicable

STN

Dialog

Questel/Orbit

Dr.Link

Lexis/Nexis.

Sequence Systems

WWW/Internet

Other (specify):

=> fil hcaplus
 FILE 'HCAPLUS' ENTERED AT 13:45:48 ON 07 MAY 2002
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FILE COVERS 1907 - 7 May 2002 VOL 136 ISS 19
 FILE LAST UPDATED: 6 May 2002 (20020506/ED)

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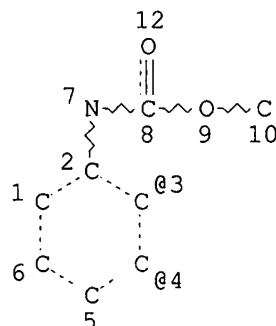
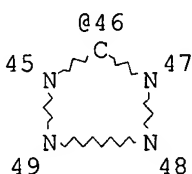
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=> d stat que

L3 STR

G4^G2^G3
 13 14 15

O≡C~O
 42 @43 44



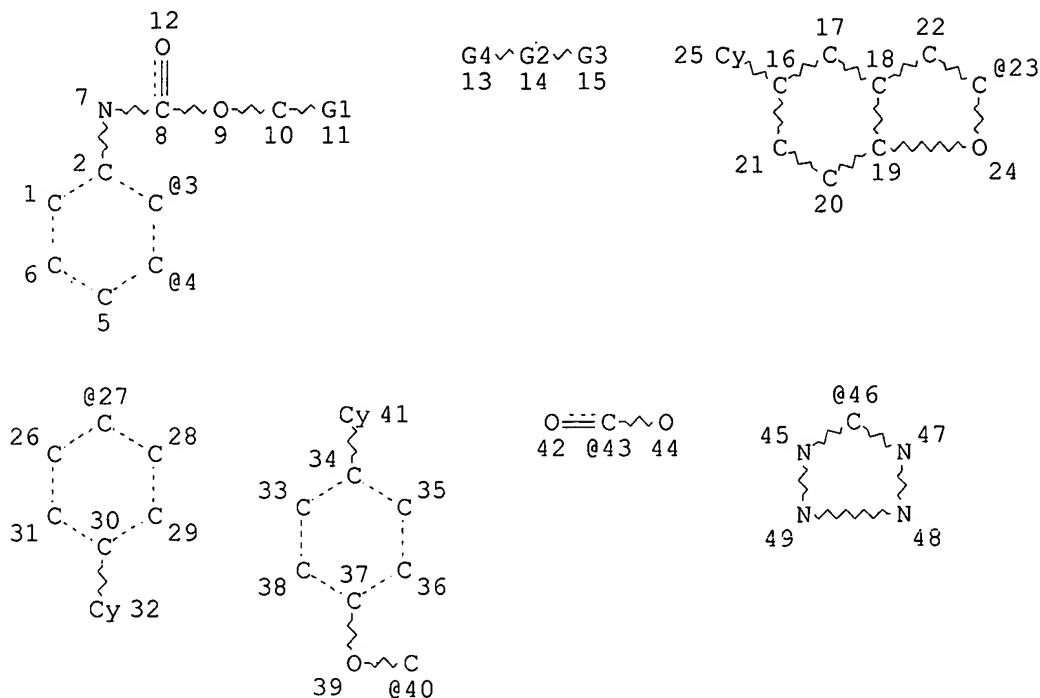
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 VAR G4=3/4
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 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L5 1208 SEA FILE=REGISTRY SSS FUL L3

L8 STR



VAR G1=23/27/40

REP G2=(0-3) C

VAR G3=43/46

VAR G4=3/4

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 49

STEREO ATTRIBUTES: NONE

L9 1 SEA FILE=REGISTRY SUB=L5 SSS FUL L8

L10 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L9

=>

=>

=> d ibib abs hitrn l10 1

L10 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1980:6533 HCAPLUS

DOCUMENT NUMBER: 92:6533

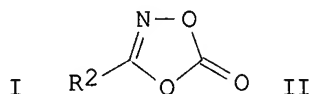
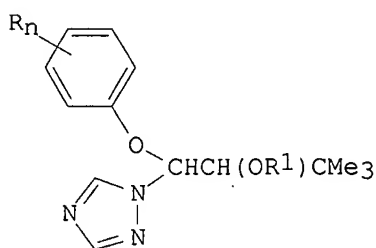
TITLE: Fungicidal carbamoyltriazolyl-O,N-acetals

INVENTOR(S): Buechel, Karl Heinz; Kraemer, Wolfgang; Brandes, Wilhelm

PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 22 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2800544	A1	19790719	DE 1978-2800544	19780107
CA 1094258	A1	19810127	CA 1977-272661	19770225
US 4237142	A	19801202	US 1978-971291	19781220
EP 3049	A2	19790725	EP 1978-101848	19781223
EP 3049	B1	19800820		
EP 3049	A3	19790808		
R: BE, CH, DE, FR, GB, IT, NL, SE				
RO 75739	P	19810228	RO 1978-96067	19781227
SU 910108	A3	19820228	SU 1979-2706202	19790103
CS 204043	P	19810331	CS 1979-134	19790104
DK 7900046	A	19790708	DK 1979-46	19790105
JP 54100377	A2	19790808	JP 1979-72	19790105
BR 7900048	A	19790814	BR 1979-48	19790105
ES 476617	A1	19791101	ES 1979-476617	19790105
ZA 7900045	A	19800130	ZA 1979-45	19790105
DD 141256	C	19800423	DD 1979-210358	19790105
AT 7900107	A	19810115	AT 1979-107	19790105
AT 363723	B	19810825		
PL 115653	B1	19810430	PL 1979-212674	19790105
CA 1113945	A1	19811208	CA 1979-319159	19790105
HU 23086	O	19820830	HU 1979-BA3745	19790105
HU 180673	B	19830429		
IL 56378	A1	19830515	IL 1979-56378	19790105
AU 7943183	A1	19790712	AU 1979-43183	19790108
AU 517276	B2	19810716		
PRIORITY APPLN. INFO.:			DE 1978-2800544	19780107
GI				



AB The title compds. I [R = halogen, alkyl, alkoxy, esterified CO₂H, (un)substituted Ph, PhO, or phenylalkyl, NH₂, NO₂, CN, etc; R₁ = R₂CO; R₂ = alkyl, halo- or alkoxyalkyl; esterified CO₂H, substituted Ph, alkylsulfonylalkenylcarbamoyl; n = 0-5] were prepd. by the reaction of I (R₁ = H) with R₂NCO or II and tested for fungicidal activity. Thus, I (R_n = 4-Ph, R₁ = H) reacted with MeOCH₂NCO in THF to give I (R_n = 4-Ph, R₁ = MeOCH₂NHCO).

IT **72013-94-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

=> fil reg

FILE 'REGISTRY' ENTERED AT 13:46:05 ON 07 MAY 2002

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STRUCTURE FILE UPDATES: 5 MAY 2002 HIGHEST RN 411206-65-0

DICTIONARY FILE UPDATES: 5 MAY 2002 HIGHEST RN 411206-65-0

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

=>

=> d ide can l9 tot

L9 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 72013-94-6 REGISTRY

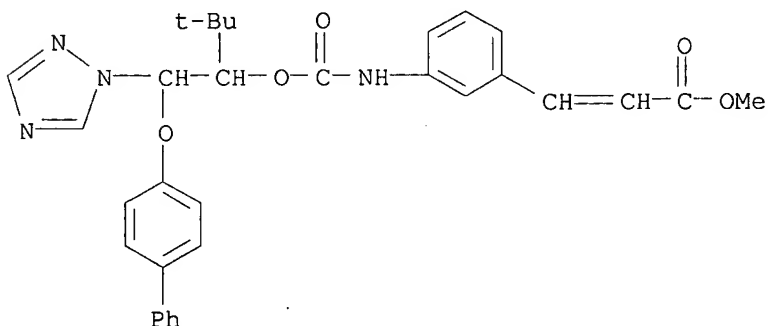
CN 2-Propenoic acid, 3-[3-[[[1-[(1,1'-biphenyl)-4-yloxy]-1H-1,2,4-triazol-1-ylmethyl]-2,2-dimethylpropoxy]carbonyl]amino]phenyl]-, methyl ester (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C31 H32 N4 O5

LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Sudhaker 10_087034

REFERENCE 1: 92:6533

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 13:47:47 ON 07 MAY 2002

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FILE COVERS 1907 - 7 May 2002 VOL 136 ISS 19

FILE LAST UPDATED: 6 May 2002 (20020506/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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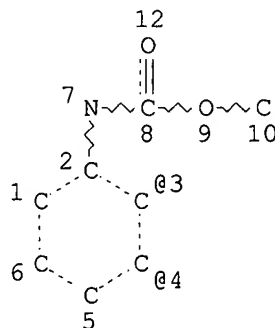
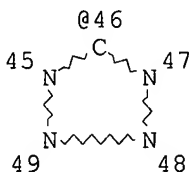
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=> d stat que 115

L3 STR

G4~G2~G3
13 14 15

O=C~O
42 @43 44



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VAR G4=3/4

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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

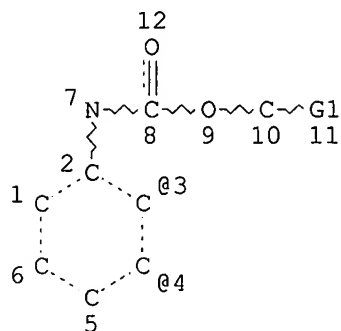
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NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

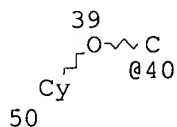
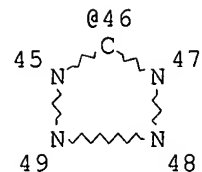
L5 1208 SEA FILE=REGISTRY SSS FUL L3

L6 STR



G4~G2~G3
13 14 15

O=C~O
42 @43 44



VAR G1=CY/40

REP G2=(0-3) C

VAR G3=43/46

VAR G4=3/4

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

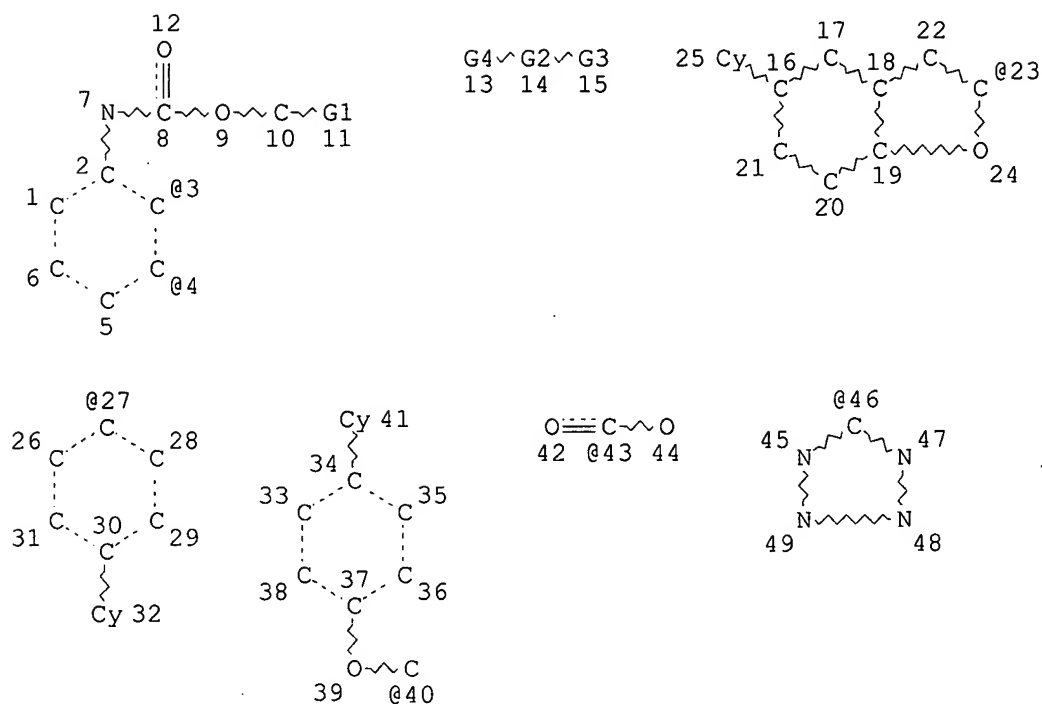
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NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

L7 247 SEA FILE=REGISTRY SUB=L5 SSS FUL L6

L8 STR



VAR G1=23/27/40

REP G2=(0-3) C

VAR G3=43/46

VAR G4=3/4

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 49

STEREO ATTRIBUTES: NONE

L9	1	SEA	FILE=REGISTRY	SUB=L5	SSS	FUL	L8
L10	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L9
L11	1022	SEA	FILE=REGISTRY	ABB=ON	PLU=ON		PROSTAGLANDIN?
L12	176	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L7
L13	86672	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L11 OR PROSTAGLANDIN?
L14	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L12 AND L13
L15	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L14 NOT L10

=> d ibib abs hitrn l15 1-2

L15 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:524350 HCAPLUS

DOCUMENT NUMBER: 125:221883

TITLE: Solid phase and combinatorial synthesis of benzodiazepines on a solid support

INVENTOR(S): Ellman, Jonathan A.

PATENT ASSIGNEE(S): The Regents of the University of California, USA

SOURCE: U.S., 43 pp., Cont.-in-part of U.S. 5,288,514.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5545568	A	19960813	US 1993-161677	19931202
US 5288514	A	19940222	US 1992-944469	19920914

PRIORITY APPLN. INFO.: US 1992-944469 19920914

AB Methods, compns., and devices for synthesizing combinatorial libraries of various useful compds., such as benzodiazepines, **prostaglandins**, .beta.-turn mimetics and glycerol-derived drugs is described. In order to expediently synthesize such combinatorial libraries of derivs. based upon these core structures, a general methodol. for the solid phase synthesis of these derivs. is also provided. This disclosure thus also describes an important extension of solid phase synthesis methods to nonpolymeric org. compds.

IT 155505-57-0P 155505-71-8P 155505-74-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (solid phase and combinatorial synthesis of benzodiazepines on a solid support)

L15 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:409430 HCAPLUS
 DOCUMENT NUMBER: 121:9430
 TITLE: Solid phase and combinatorial synthesis of benzodiazepine compounds on a solid support
 INVENTOR(S): Ellman, Jonathan A.
 PATENT ASSIGNEE(S): Regents of the University of California, USA
 SOURCE: U.S., 25 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5288514	A	19940222	US 1992-944469	19920914
WO 9406291	A1	19940331	WO 1993-US8709	19930913

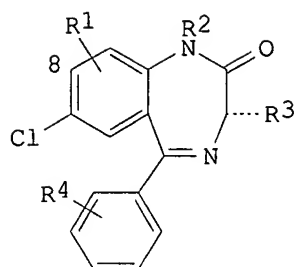
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

US 5545568	A	19960813	US 1993-161677	19931202
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PRIORITY APPLN. INFO.: US 1992-944469 19920914

GI



I

AB The invention provides a rapid approach for combinatorial synthesis and screening of libraries of derivs. of therapeutically important classes of compds. such as benzodiazepines, **prostaglandins**, and .beta.-turn mimetics. A general methodol. for the solid-phase synthesis of these derivs. is provided. For example, in the case of 1,4-benzodiazepines such as I [R1 = H, 8-CO2H; R2 = H, Me, Et, allyl, CH2Ph; R3 = Me, CH2C6H4OH-4, iso-Pr, CH2CO2H, CH2Ph, (CH2)4NH2; R4 = H, 4-OH], a substituted, N-FMOC-protected 2-aminobenzophenone is coupled via another functional group to a solid support, preferably by a cleavable linker. After deprotection of N, the bound aminobenzophenone reacts with an FMOC-protected amino acid (natural or unnatural), followed by base-catalyzed deprotection of the FMOC group and acid-catalyzed cyclization, to give a benzodiazepinone deriv. This may undergo further N-alkylation. By varying the aminobenzophenones, amino acids, and alkylating agents, using, e.g., pin-based, bead-based, or light-directed synthetic techniques, a plurality of benzodiazepines can be prepd. simultaneously.

IT 155505-71-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and coupling of, with resin, in solid-phase benzodiazepine synthesis)

IT 155505-57-0P 155505-71-8DP, aminomethyl resin-bound
155505-74-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in solid-phase benzodiazepine synthesis)

=>

=> select hit rn 115 1-2

E1 THROUGH E3 ASSIGNED

=> fil reg

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STRUCTURE FILE UPDATES: 5 MAY 2002 HIGHEST RN 411206-65-0

DICTIONARY FILE UPDATES: 5 MAY 2002 HIGHEST RN 411206-65-0

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> s e1-e3

1 155505-71-8/BI
 (155505-71-8/RN)

1 155505-57-0/BI
 (155505-57-0/RN)

1 155505-74-1/BI
 (155505-74-1/RN)

L16 3 (155505-71-8/BI OR 155505-57-0/BI OR 155505-74-1/BI)

=> d ide can l16 1-3

L16 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2002 ACS

RN **155505-74-1** REGISTRY

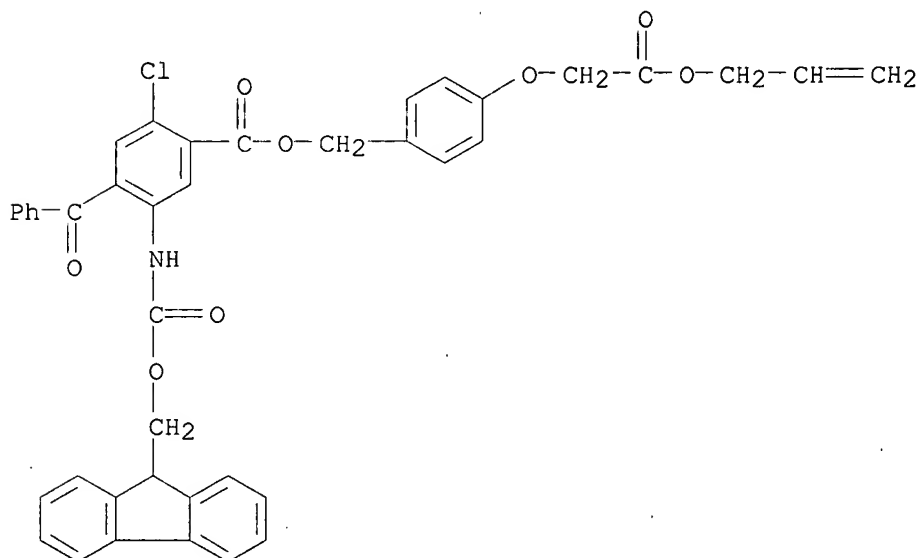
CN Benzoic acid, 4-benzoyl-2-chloro-5-[[(9H-fluoren-9-ylmethoxy)carbonylamino]-, [4-[2-oxo-2-(2-propenyloxy)ethoxy]phenyl]methyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C41 H32 Cl N O8

SR CA

LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:221883

REFERENCE 2: 121:9430

L16 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2002 ACS

RN 155505-71-8 REGISTRY

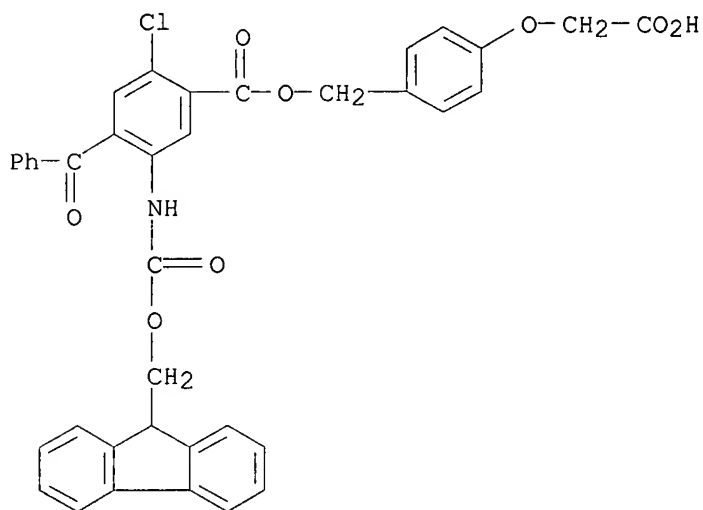
CN Benzoic acid, 4-benzoyl-2-chloro-5-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-, [4-(carboxymethoxy)phenyl]methyl ester (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C38 H28 Cl N O8

SR CA

LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:221883

REFERENCE 2: 121:9430

L16 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2002 ACS

RN 155505-57-0 REGISTRY

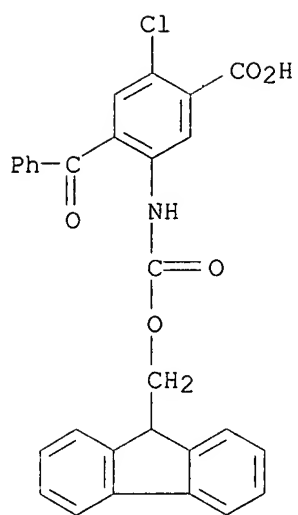
CN Benzoic acid, 4-benzoyl-2-chloro-5-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C29 H20 Cl N O5

SR CA

LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:221883

REFERENCE 2: 121:9430

=> fil hcaplus
 FILE 'HCAPLUS' ENTERED AT 13:49:12 ON 07 MAY 2002
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FILE COVERS 1907 - 7 May 2002 VOL 136 ISS 19
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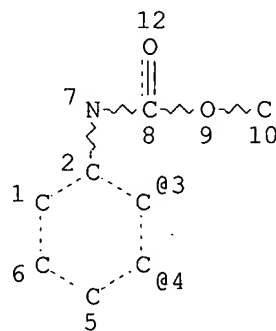
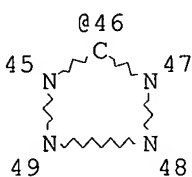
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=> d stat que 120
 L3 STR

G4~G2~G3
 13 14 15

O=C~O
 42 @43 44



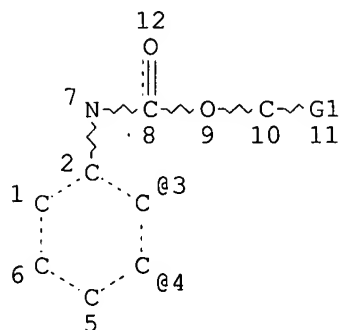
REP G2=(0-3) C
 VAR G3=43/46
 VAR G4=3/4
 NODE ATTRIBUTES:
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

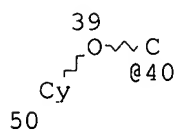
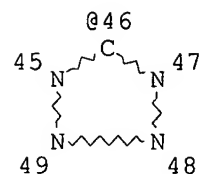
L5 1208 SEA FILE=REGISTRY SSS FUL L3

L6 STR



G4~G2~G3
13 14 15

O=C~O
42 @43 44



VAR G1=CY/40

REP G2={0-3} C

VAR G3=43/46

VAR G4=3/4

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

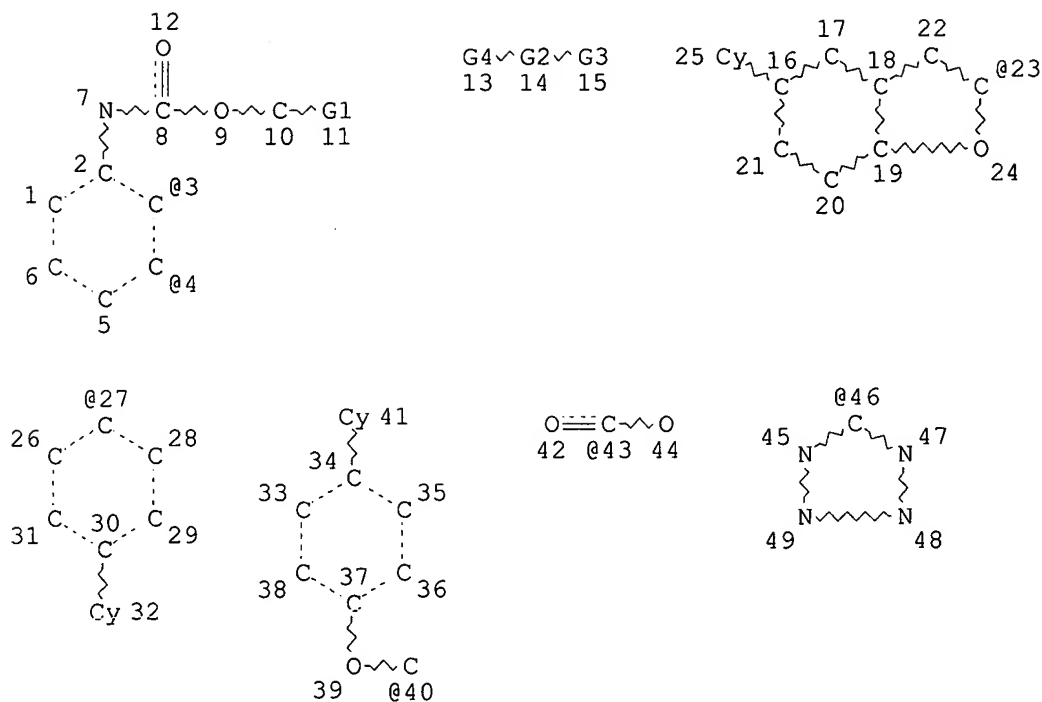
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

L7 247 SEA FILE=REGISTRY SUB=L5 SSS FUL L6

L8 STR



VAR G1=23/27/40

REP G2=(0-3) C

VAR G3=43/46

VAR G4=3/4

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 49

STEREO ATTRIBUTES: NONE

L9	1	SEA	FILE=REGISTRY	SUB=L5	SSS	FUL	L8
L10	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L9
L11	1022	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	PROSTAGLANDIN?	
L12	176	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L7
L13	86672	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L11 OR PROSTAGLANDIN?	
L14	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L12 AND L13	
L15	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L14 NOT L10	
L17	961	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L5 NOT (L7 OR L9)	
L18	509	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L17
L19	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L18 AND L13	
L20	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L19 NOT L15	

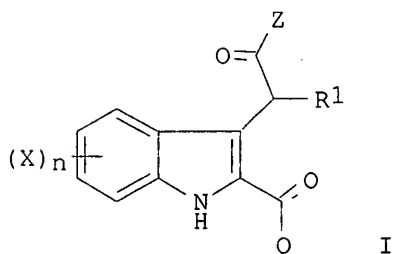
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L20 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1999:451281 HCAPLUS
 DOCUMENT NUMBER: 131:102195
 TITLE: Preparation of 2,3-Substituted indoles as COX-2 inhibitors
 INVENTOR(S): Nakao, Kazunari; Stevens, Rodney William; Kawamura, Kiyoshi; Uchida, Chikara; Koike, Hiroki; Caron, Stephane
 PATENT ASSIGNEE(S): Pfizer Pharmaceuticals Inc., Japan; Pfizer Inc.
 SOURCE: PCT Int. Appl., 347 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9935130	A1	19990715	WO 1998-IB2065	19981218
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2316863	AA	19990715	CA 1998-2316863	19981218
AU 9915005	A1	19990726	AU 1999-15005	19981218
BR 9813124	A	20001010	BR 1998-13124	19981218
EP 1045833	A1	20001025	EP 1998-959082	19981218
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO			
JP 2002500217	T2	20020108	JP 2000-527531	19981218
TW 436482	B	20010528	TW 1998-87120865	19981222
ZA 9900011	A	20000704	ZA 1999-11	19990104
NO 2000003451	A	20000901	NO 2000-3451	20000704
PRIORITY APPLN. INFO.:			WO 1998-IB3	A 19980105
			WO 1998-IB2065	W 19981218
OTHER SOURCE(S):		MARPAT 131:102195		
GI				



AB Title compds. [I or the pharmaceutically acceptable salts thereof; wherein

Z is OH, C1-6 alkoxy, -NR₂R₃ or heterocycle; Q is selected from the following: (a) an optionally substituted Ph, (b) an optionally substituted 6-membered monocyclic arom. group contg. one, two, three or four nitrogen atom(s), (c) an optionally substituted 5-membered monocyclic arom. group contg. one heteroatom selected from O, S and N and optionally contg. one, two or three nitrogen atom(s) in addn. to said heteroatom, (d) an optionally substituted C3-7 cycloalkyl and (e) an optionally substituted benzofused heterocycle; R₁ is hydrogen, C1-4 alkyl or halo; R₂ and R₃ are independently hydrogen, OH, C1-4 alkoxy, C1-4 alkyl or C1-4 alkyl substituted with halo, OH, C1-4 alkoxy or CN; X is independently selected from H, halo, C1-4 alkyl, halo-substituted C1-4 alkyl, OH, C1-4 alkoxy, halo-substituted C1-4 alkoxy, C1-4 alkylthio, NO₂, NH₂, di-(C1-4 alkyl)amino and CN; and n is 0, 1, 2, 3 and 4] are prepd. as COX-2 inhibitors which provide pharmaceutical compns. useful for the treatment of a medical condition in which **prostaglandins** are implicated as pathogens. Thus, title compd. I (R₁ = H; Z = OEt; Q = C₆H₅; (X)_n = 6-C1) was prepd. from 4-chloro-2-nitrobenzaldehyde, formic acid, and triphosgene in 5 steps via cyclization.

IT 231295-97-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 2,3-substituted indoles. as COX-2 inhibitors)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:424220 HCAPLUS

DOCUMENT NUMBER: 129:95327

TITLE: Preparation of sulfonamide and carboxamide derivatives as drugs

INVENTOR(S): Ohuchida, Shuichi; Nagao, Yuuki

PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan; Ohuchida, Shuichi; Nagao, Yuuki

SOURCE: PCT Int. Appl., 305 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9827053	A1	19980625	WO 1997-JP4593	19971212
W: AU, CA, CN, HU, JP, KR, MX, NO, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9854115	A1	19980715	AU 1998-54115	19971212
AU 733493	B2	20010517		
EP 947500	A1	19991006	EP 1997-947925	19971212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
CN 1247529	A	20000315	CN 1997-181861	19971212
ZA 9711336	A	19980625	ZA 1997-11336	19971217
KR 2000057576	A	20000925	KR 1999-705335	19990615
NO 9902935	A	19990816	NO 1999-2935	19990616
PRIORITY APPLN. INFO.:			JP 1996-353818	A 19961218
			JP 1997-305055	A 19971021
			WO 1997-JP4593	W 19971212

OTHER SOURCE(S): MARPAT 129:95327

GI For diagram(s), see printed CA Issue.

AB The title compds. (I; rings A and B represent each a carbocycle or a

heterocycle; Z1 represents COR1, CH:CHCOR1, etc.; R1 represents OH, C1-4 alkoxy, etc.; Z2 represents H, alkyl, etc.; Z3 represents a single bond or alkylene; Z4 represents SO2 or CO; Z5 represents alkyl, Ph, a heterocycle, etc.; R2 represents CONR8, O, S, etc.; R8 represents H, C1-4 alkyl; R3 represents H, alkyl, halo, CF3, etc.; R4 represents H, optionally substituted alkyl, etc.; n, t = 1-4 are prepd. I bind to **prostaglandin E2 (PGE2)** receptors and exert an antagonism. I have the effects of inhibiting uterine muscle contraction, analgesia, inhibiting digestive tract movement, hypnosis, enlarging vesical capacity, contracting the uterine, promoting the digestive tract movement, suppressing the secretion of gastric hydrochloric acid, lowering blood pressure, or diuresis. Thus, compd. (II; W = Me) was treated with aq. NaOH and followed by aq. HCl to give the title compd. II (W = H), which showed K_i of 0.099 μM against PGE2 receptors.

IT 209688-24-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of sulfonamide and carboxamide derivs. as drugs)

=> select hit rn 120 1-2
E4 THROUGH E5 ASSIGNED

=> fil reg
FILE 'REGISTRY' ENTERED AT 13:49:35 ON 07 MAY 2002
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DICTIONARY FILE UPDATES: 5 MAY 2002 HIGHEST RN 411206-65-0

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

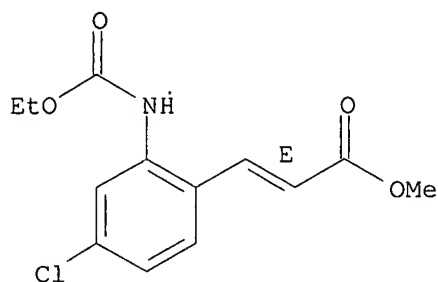
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1 209688-24-4/BI
(209688-24-4/RN)
1 231295-97-9/BI
(231295-97-9/RN)
L21 2 (209688-24-4/BI OR 231295-97-9/BI)

=> d ide can 121 1-2

L21 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2002 ACS
RN 231295-97-9 REGISTRY
CN 2-Propenoic acid, 3-[4-chloro-2-[(ethoxycarbonyl)amino]phenyl]-, methyl
ester, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C13 H14 Cl N O4
SR CA

LC STN Files: CA, CAPLUS

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:102195

L21 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2002 ACS

RN **209688-24-4** REGISTRY

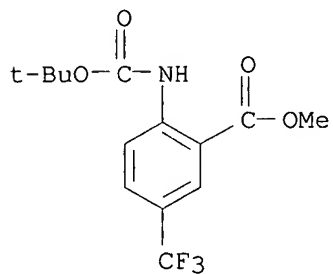
CN Benzoic acid, 2-[[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H16 F3 N O4

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:95327